Appendix 1. Summaries of Individual Calibration Papers Cited in Chapter 2

The following paragraphs provide a summary of each of the 35 articles listed in Table 2-1, including relevant conclusions of the papers' authors.

Barrett (1995) examined the leaching of triasulfuron residues in a loamy sand in Kansas using field results and PRZM modeling. The author concluded "Modeling of triasulfuron movement with PRZM resulted in a simulation that predicted accurately the time of appearance of triasulfuron residues at lower depths (ca. 60 days) and the mass flux (nearly 10% of applied moving to shallow ground water within 6 months after application), but underestimated dispersion and therefore overestimated peak concentrations in shallow ground water by a factor of two or three." The author noted that PRZM does not simulate preferential flow in structured soils and indicated "Given the uncertainty of extrapolating persistence and mobility data for each wheat herbicide from other soils to the test site, one cannot with confidence predict how much of each compound would leach under a given scenario. The PRZM modeling results do, however, give us a very good indication about which herbicides are more or less likely to leach in significant amounts. Therefore, PRZM does show promise to be used as a tool to place field monitoring data for a pesticide in perspective by simulating other weather conditions or cultural practices at the test site and by simulating leaching of other pesticides."

Cai et al. (1993) examined the leaching of aldicarb residues from a banded application in a cotton field with sandy loam soil in Jiangsu province, China and compared the results to predictions made by the PRZM model (v 1). The model appeared to under predict the concentration in the soil during the early samplings (a factor of 2-3 at 30 days), however the authors noted that: "This may be due to the fact that the field soil sampling core was collected immediately beneath the aldicarb application point, so that the aldicarb residue concentration cannot represent the field-average concentration. If converted to "field-average concentrations, ..., the predicted results would be close to the measured field concentrations. With increasing sample depth and time, the two results tend to be more consistent. This is due to aldicarb diffusing and moving downward in the form of a pyramid beneath the application point with lateral dispersion producing a more even aldicarb distribution in the soil profile."

Carsel et al. (1985) examined the use of the PRZM model (v 1) to predict the leaching of aldicarb residues in New York. A simulation was first performed which did not use any site specific data and thus was run as a "calibration-free" assessment. The model accurately predicted the maximum concentration within less than 10% of the measured value, but overestimated the amount of movement through the soil. A series of calibration runs was performed on the individual soil core results and the average of the soil core results. In all three cases increasing the adsorption coefficient to twice the uncalibrated values and making small adjustments in the degradation rates resulted in predictions of peak concentrations within less than 10% of the measured values and all other values within a factor of two to three.

Carsel et al. (1986) compared PRZM (v 1) predictions with measured soil concentrations of metalaxyl from sites in Florida and Maryland. The model over predicted the amount of leaching early in the study at the Florida site (26 days after application) but provided an excellent fit (predicted values were within 30% of measured values) at 55 and 85 days after application. At the Maryland site both the observed and the predicted values indicated that residues remained in the top 15 cm of the soil. The predicted concentrations were within a factor of two of the observed values, with a general over prediction of the concentrations.

Dibbern and Pestemer (1992) examined the ability of the GLEAMS, PRZM, CALF, LEACHM, SESOIL, EQUI models to describe the leaching of terbuthylazine through a loamy soil in Germany. The GLEAMS model greatly over predicted the amount of leaching, as indicated by the depth of the peak (predicted peak at 15 - 20 cm versus observed at 0-3 cm), and greatly under predicted the concentration of the residues in the upper layers. The PRZM model slightly over predicted the movement (predicted peak at 3 - 6 cm versus observed at 0-3), and was able to predict lower concentrations within a factor of 2 - 3, except for a measure value at 24-30 cm, which was three times greater than the measured value at 18-24 cm.

Dowd et al. (1993) compared the dissipation of lindane residues in a forest in Georgia with predicted values from the PRZM model (v 1). The PRZM model was not able to accurately predict the measured concentrations below the top 10 cm. The authors felt that this was probably due to the inability to model preferential flow, which is probably a very important pathway in water movement in the highly structured soils commonly encountered in forests.

Flori et al. (1993) examined the leaching of metamitron, chloridazon, ethofumesate and lenacil residues in a field in the Po Valley of Italy using PRZM (v 1). The authors noted that the soil horizon thickness parameter (THKNS) had a major effect on predicting the mobility and persistence of the compounds.

Hegg et al. (1988) studied the leaching of aldicarb residues in a Dothan loamy sand in South Carolina. The field data and the predictions of PRZM (v 1) were in good agreement since they indicated that detectable residues would only be found in the top 0.6 m of soil. The authors indicated that it would not be appropriate to compare predicted and observed residue concentrations since the degradation rate used in the simulation was taken from the field results.

Jones et al. (1983) examined the leaching of aldicarb residues at two sites in Florida using the PRZM model (v 1). PRZM underestimated the depth of the peak at an early time point, 2 weeks after application (approximately 60 cm versus 160 cm), but only slightly underestimated the peak locations at 6 and 11 weeks after application (approximately 210 cm versus 260 cm and 225 cm versus 260 cm, respectively). The authors indicated that these slight under predictions were due to dispersion.

Jones et al. (1986) compared the predicted leaching of aldicarb and aldoxycarb residues using the PRZM model (v 1) with field data from Arizona, California, Florida, Indiana, Maine, Michigan, Nebraska, New York, North Carolina, South Carolina, Virginia, Washington and Wisconsin. The authors noted "In this paper, degradation rates were calculated from the measured residue concentrations. Thus comparison of field and predicted degradation rates are not appropriate." The maximum leaching depth, defined as the depth below which the average concentration was less than the sensitivity of the analytical method, was compared for 34 field plots. In most cases where the measured leaching depth was greater than 60 cm the model tended to over predict the depth of leaching, although the over prediction was generally less than 50%, i.e. observed depth of 2 m versus a calculated depth of 3 m. There were two sites, in AZ and CA, where this did not hold; both used flood or furrow irrigation. The authors concluded: "Because PRZM does a relatively good job of predicting the leading edge of the residue profile, assessments based on predictions of the maximum leaching depth are appropriate. However, because the model is often less accurate in predicting concentration profiles especially without calibration of parameters, assessments based on soil residue concentrations as a function of time and depth will be much less reliable. (The variability of soil data also makes field measurements of concentration profiles difficult.) Estimates of the amount of material moving past a specified depth will usually also be reasonably accurate (the model will again usually tend to overestimate the amount of material) since these estimates are not highly dependent on the shape of the concentration profile. Therefore, use of PRZM should be limited to assessing whether a pesticide will reach ground water in a specific situation and if so, how long it will take the residues to reach the water table and what percent of the applied material will enter ground water under the specified conditions. Usually, an acceptable risk assessment will need to address only these three issues so PRZM is a useful and appropriate tool."

Jones et al. (1987) investigated the leaching of aldicarb residues through sandy soil in Nebraska and compared the measured values with those predicted by PRZM (v 1). The authors note that "Because the soil cores were taken from the middle of treated bands whereas the simulated concentrations are field average concentrations and because the degradation rate used in the simulation was estimated from the field data, it is not appropriate to closely compare predicted and simulated residue concentrations." The model predictions were conservative in that they tended to slightly over predict the movement of aldicarb residues, with the predicted values being within a factor of 2 - 3 of the measured values.

Khan and Green (1988) modeled the leaching of dibromochloropropane (DBCP) in two pineapple fields in Hawaii. PRZM (v 1) correctly predicted the depth of the peak concentration and the general shape of the concentration profile with depth, although it could not predict the magnitude of the concentration. The authors indicated that they did not expect PRZM to accurately calculated the concentrations of DBCP in soil because PRZM does not take into account volatilization, which is a major dissipation mechanism for DBCP (later versions of PRZM do include volatilization).

Leonard et al. (1990) conducted studies designed to validate the GLEAMS model using field data from Georgia on fenamiphos and its sulfoxide and sulfone metabolites. Estimated values were used for the hydrology and erosion parameters as well as estimated degradation and adsorption values for the three compounds. The authors concluded "GLEAMS-simulated mass of fenamiphos, fenamiphos sulfoxide and fenamiphos sulfone in the root zone compared favorably with field data within the variability of the data. Simulated and observed concentrations with depth in the soil at selected dates also closely corresponded. Results of the limited validation give confidence that the model component is performing as conceptualized." The predictions of the GLEAMS model slightly overestimated the total amount of fenamiphos and its metabolites in the soil profile but were within the confidence intervals of the measured data.

Loague (1992) calibrated the PRZM model (v 1) for the leaching of ethylene dibromide (EDB) in a pineapple field on Oahu, Hawaii using two years of data. The authors examined several methods to compare the results of measured values with modeling results. These include such factors as: (1) total mass; (2) center of mass; (3) peak concentration; (4) time for a specific concentration to leach to a certain depth; (5) depth to peak concentration; and (6) depth to the leaching front. They concluded that if they used the data from one year to calibrate the model, the results were poor for the other year. The authors concluded that the poor fit was not surprising due to the deep leaching being simulated and potential problems with the data sets.

Loague et al. (1989a) used PRZM (v 1) to evaluate the leaching of ethylene dibromide (EDB) in two pineapple plantations in Hawaii. This paper is the first of a series of three papers. The results of the comparisons with the data are described in the later two papers in the series, which have also been summarized.

Loague et al. (1989b) examined the leaching of 1,2-dibromo-3-chloropropane (DBCP), ethylene dibromide (EDB), and 1,2,3-trichloropropane (TCP) in structured soils in Hawaii using the PRZM model (v 1). The authors of the paper recognized they were attempting to use the model under conditions for which the model was not designed: "PRZM was not designed to simulate pesticide movement over the extended depths included in this study.. The structure of PRZM is best suited to areas that are dominated by deep, well-drained sands where the water table is near the surface. These conditions are not met for the pineapple fields in Hawaii. With this limitation in mind, we have applied PRZM beyond its intended range to determine if the model can provide reasonable estimates of pesticide mobility over multiyear periods." In addition to the limitations involving the structure and depths of the soil, additional adjustments had to be made because of the high degree of volatility of the three compounds studied. Despite these severe limitations, when adjustments were made for degradation and/or volatilization the predicted peak concentrations of EDB in soil were within a factor of 2-4 of the measured concentrations, with the model overestimating the depth of leaching. Similar results were found for both DBCP and TCP in the top 12 meters of the soil, but the model greatly over predicted the concentrations from 12 - 20 meters. The authors concluded "In this paper we show that deep leaching of DBCP, EDB, and TCP is reasonably well predicted with PRZM at a single well-characterized site. We cannot, however, suggest that PRZM should be used in Hawaii for decision/management purposes until further testing has been conducted."

Loague et al. (1995) used the PRZM model (v 1) to examine the leaching of bromide, chlorpyrifos and fenamiphos in two sites in Hawaii. PRZM was generally able to model the movement of bromide and generally gave results that were within a factor of two of the measured results. In one of the test plots the model was not able to predict the upward movement of bromide by capillary rise. The authors concluded "The results of this study show that PRZM simulated near-surface transport with some degree of accuracy. Based upon analysis of residual errors, coupled with qualitative graphical comparisons, it was evident, however, that PRZM could not be rigorously validated with the available data."

Lorber and Offutt (1986) examined the use of PRZM (v 1) in predicting leaching of aldicarb residues in North Carolina and Wisconsin as an assessment tool for predicting the potential for ground water contamination. A comparison of observed versus predicted values for aldicarb residues at three sites with nine distinct scenarios was excellent, with observed versus predicted values generally within a factor of 2 and always within a factor of 5. This paper also provides important information on factors to consider when calibrating the model with field data.

Mueller (1994) modeled the leaching of dichlorprop and bentazon through lysimeters in Sweden using PRZM (v 1) and compared the results to field data. Bentazon movement was examined in a sand and a clay while dichlorprop movement was studied in clay, sand and loam soils. There were two significant modifications made to two sets of hydrologic parameters. "First, the initial soil-water content was adjusted to coincide the time of first water discharge between simulated and actual data. In essence the model assumed the profile was not saturated, and that as water was loaded onto the top of the column it slowly filled the soil until each layer was filled and then water discharge would begin." Secondly, "... the difference between field capacity (FC) and permanent wilting point (PWP) was adjusted in each soil horizon." When these two modifications were made there was an excellent agreement between the measured and calculated volume of water leaching from all five soils during one year. The loss of bentazon from the soil columns was accurately predicted over the year of the study, with, based on an examination of the graphs in the paper, less than a 10% difference between the observed and predicted values after one year. For dichloroprop there was a significant difference between observed and predicted values, with the observed values being much higher starting at about 200 days after treatment. The authors indicated "The laboratory incubation experiments indicate near-complete herbicide degradation in less than 5 days; yet the lysimeters were discharging dichlorprop at 300 days after initial application. One fertile research area to help explain this would be to examine the effect of temperature on herbicide degradation. The combined effect of lower microbial activity and lower soil temperature in subsurface zones (below approximately 30 cm) could greatly reduce dichlorprop degradation, thus explaining the discharge results. However, the PRZM simulations were performed assuming no dichlorprop degradation in subsurface zones, and these simulations did not predict any dichlorprop discharge."

Mueller et al. (1992) examined the ability of the PRZM (v 1) and GLEAMS (v 1.8.55) models to predict the leaching of alachlor, metribuzin and norflurazon in a loamy sand soil in Georgia. Both models accurately predicted the observed concentrations of norflurazon in the soil profile with the predicted values equivalent to the observed values at 84 days. For alachlor and metribuzin, both models accurately predicted the observed concentrations in the soil profile within the first 20 days, then over predicted the movement through the soil profile. For metribuzin, the observed concentrations were within a factor of 3 for the first 20 days and within a factor of 4 by day 40, the last day at which measured values were above the limit of detection. For alachlor, the observed concentrations were within a factor of 4 for the first 20 days and within a factor of 7 by day 40, the last day at which measured values were above the limit of detection. One of the authors' conclusions is "We have attempted to assess the accuracy of these two models under a certain set of conditions. We could take these data and "calibrate" the model by changing model input parameters to improve model accuracy, but this would lead to artificial model accuracy. To go forth and subsequently use the calibrated models (with altered input data sets) in an attempt to simulate the effects of different environmental and management scenarios would be equivalent to using the uncalibrated model because the model's performance was examined under a single set of conditions. Each different set of conditions would require a separate validation experiment."

Nicholls (1994) studied the movement of bentazon through lysimeters containing a sand using the PRZM and CALF models. PRZM (v 1) was able to accurately predict the total amount of leachate produced over 325 days and the total amount of bentazon leached. Unfortunately the model over predicted the amount of leachate produced early in the experiment but this was due to the modelers not simulating the presence of a crop in the lysimeter, which would have increased the amount of evapotranspiration, and not simulating the two months of freezing conditions, which allowed for the model to predict leaching even though this did not occur under the experimental conditions. Bentazon appeared in the leachate earlier than predicted by the models. The authors indicated: "Results of simulations were sensitive to values of sorption and rates of degradation chosen for the soil below the cultivation layer. It may have been possible to improve the fit between measured and simulated values by finely adjusting such input but in the absence of measured data this would not have been sufficiently informative to be justifiable."

Parrish et al. (1992) used the PRZM (v 2) and AGGR models to examine the leaching of aldicarb, metolachlor and bromide in a four year field study in the Dougherty Plain area of southwestern Georgia. For metolachlor, which was studied for three years, the predicted values using PRZM were within a factor of 2 of the measured value for over 90% of the measured values and within a factor of 5 for all of the measured values (up to 10 per year). The few times when the predicted value was greater than twice the measured value occurred when the observed values were very small. For aldicarb, which was studied for four years, there was more variability in the comparisons. The predicted values using PRZM were within a factor of 2 of the measured value for 60 to 100% of the measured values and within a factor of 5 for 82-100% of the measured values (up to 15 per year). The model tended to over predict the movement of aldicarb through the soil profile, which lowered the goodness of fit, especially when very low measured residues were detected. Modeling the movement of bromide was more difficult. The authors concluded "The lack of mass balance in bromide suggests that preferential flow is a significant factor that may adversely affect the viability of advection-dispersion models for these soils. Nonetheless, both PRZM and AGGR accurately predicted bromide peak concentrations down to 1 meter, but diverged considerably thereafter by predicting deeper movement than actually occurred."

Pennell et al. (1990) examined the leaching of aldicarb and bromide through a sand in Florida using GLEAMS (v 1.8.54) and PRZM (v 1). The predicted PRZM values were within approximately 30, 45 and 70% of the measured values for bromide, aldicarb and total aldicarb related residues, respectively. GLEAMS underestimated the dissipation of bromide and total aldicarb related residues in the root zone and over predicted the solute concentrations near the soil surface.

Perry (1991) examined the leaching of atrazine, alachlor, metolachlor, trifluralin and 2,4-D residues in Kansas and compared them to results predicted by the PRZM model (v 1). The authors indicated that "The PRZM was best calibrated to the observed data for the three soil types by treating the sand-and-silt fraction as sand and adjusting the organic-carbon content by a factor of 0.1. These adjustments provided the best overall correlation between observed and modeled values. These adjustments are simple and can be justified as corrections by the fact that the PRZM does not allow for macropore flow. Increasing the half-life of the herbicide with depth and degree of saturation has been shown to occur in saturated conditions and appears to be applicable to the unsaturated regime below the root zone. These three major adjustments to the input data for the PRZM improved the correlation between observed and simulated concentrations of atrazine for the three soil types and at all depths...."

Sadeghi et al. (1995) compared the effects of conventional versus no-till management systems on the leaching of atrazine during three growing seasons in silt loam soils in Maryland, using field results and the PRZM model (v 1). The modeling results over predicted, by less than a factor of 2, the levels in the top 10 cm of the soil. The modeling was not able to predict the low concentrations, generally less than 25 ppb, detected in 10 cm increments from 20 to 50 cm. The authors concluded "Part of the inaccuracies of the PRZM predictions for the atrazine residue levels remaining in the top soils (0 to 10 cm) in both tillage systems is because some input parameters are difficult to measure accurately, and the estimation of such parameters is a possible source of error. The under estimation of atrazine residue levels remaining in the lower soil depths (20 to 30 cm), in the NT system by the model, may be due to the fact that the PRZM was not intended to consider solute transport via macropore flow processes. Consequently, the PRZM model calculations did not account for the preferential transport portion of the atrazine leachate for the top soil into the lower soil horizons."

Sauer et al. (1990) examined the leaching of atrazine and metolachlor in a field study in Wisconsin, and the movement of carbofuran and chlorpyrifos in intact soil columns. The results of the experiments were compared to results from the PRZM model (v 1). Starting after the 14 day sampling point, PRZM predicted deeper movement of atrazine residues than were observed. Similar results were found for metolachlor. One of the problems of this study was the lack of mobility of the compounds in the field, which was due to the low rainfall during the study. The author concluded: "This study indicates that PRZM can make reasonable predictions of pesticide movement in a coarse-textured soil under both moldboard plow and no-till tillage systems early in the growing season. Inclusion of input parameter values unique to the respective tillage systems for organic C content, bulk density, and dissipation rate resulted in distinctly different predictions of pesticide movement. However, the accuracy of the model predictions, especially later in the growing season, would likely have been significantly improved by the increased use of measured site-specific input parameters including pesticide adsorption coefficients and soil moisture retention characteristics for each of the soil profiles."

Shirmohammadi and Knisel (1994) examined the leaching of dichloprop and bentazon through lysimeters in Sweden using the GLEAMS model (v 2.0). It was necessary to make several major modifications to parameters dealing with hydrology since lysimeters were being modeled rather than a field scale experiment, which is what GLEAMS was designed to simulate. The experimental values showed considerable variability, with 3 of the 4 lysimeters not producing any leachate during any given sampling period. These factors make it difficult to make an accurate assessment of the ability of GLEAMS to predict measured soil concentrations in lysimeters. It was noted "that GLEAMS does not work well in cold climates because the model cannot handle partially frozen soil."

Shirmohammadi et al., (1987;1989) used the GLEAMS model to examine the leaching of atrazine, carbofuran, cyanazine, dicamba, metolachlor and simazine in no-till and conventional tillage systems in Maryland. Predicted leaching of the pesticides was compared to the results of ground water concentrations of the pesticides. With only one exception, the model predicted higher concentrations than were observed, with the predicted values ranging from 2 - 10 times the observed values. The authors noted that there were two reasons for the lack of good agreement: "First, ground water sampling activities were not correlated with storm occurrences or individual ground water recharge events. Therefore, high pesticide concentrations might have occurred that the sampling scheme ignored. Second, the maximum observed concentrations ...... were detected mostly in one specific well that was located at a lower elevation of the watershed where topography would have enhanced infiltration and resulted in a water table closer to the soil surface."

Sichani et al. (1991) compared the leaching and runoff of alachlor, atrazine, cyanazine, carbofuran and chlorpyrifos through a tiled drainage field in Indiana with predicted values using the GLEAMS model. The model was able to predict fairly well the total mass of the compounds which moved through the soil profile as well as the overall timing of the movement, except for the first observed values in the drainage after the application. For atrazine, the predicted values were less than the observed values, with the peak differences being within a factor of 2 to 4. For carbofuran, the predicted values were greater than the observed values, with the peak differences being within a factor of 2. For cyanazine, the predicted values were within a factor of 2 to 4 of the observed values. An interesting observation was made regarding the use of Koc values for these compounds. The authors used two sets of Koc values, with one set taken from the GLEAMS manual and another set of literature values from measurements taken on soils from the study area. Depending upon which set of Koc values were used, there were significant differences in the predicted losses. Table A1-1 summarizes these findings.

Table A1-1. Effect of source of Koc on runoff and leaching losses (Sichani et al., 1991).

	Koc		Runoff loss (g/ha)		Leaching loss (g/ha)	
Compound	GLEAMS Manual	Site Measured	GLEAMS Manual	Site Measured	GLEAMS Manual	Site Measured
Atrazine	160	91	29.15	15.79	0.04	0.23
Carbofuran	40	41	0.92	0.89	0.92	0.89
Cyanazine	168	97	45.53	22.00	0.05	0.29

Smith, M. C., et al. (1991) compared the leaching of atrazine, alachlor, and bromide on a Lakeland sand in Georgia using GLEAMS (v 1.8.55) and PRZM (v 2). The authors concluded "In all cases, the measured and predicted peak concentrations agreed to within an order of magnitude, and in most cases they agreed to within a factor of 2 or 3. Thus, the PRZM and GLEAMS simulated results have met the criteria for acceptance suggested by Hedden (1986). In the work presented here, PRZM and GLEAMS were essentially run in a screening mode. Many of the model parameters were selected from tables and other information contained in the model's user manual. Parameters were not optimized or calibrated to produce the best fit. At this stage of data collection and model use, it was decided to investigate how the models would perform when run without site-specific chemical properties."

Smith, W. N., et al. (1991) compared the leaching of atrazine through intact soil cores in the laboratory with predictions made using the PRZM model (v 1). It was necessary to calibrate the model in order to obtain the proper hydrologic balance. The ability of the model to predict the concentration of atrazine in the leachate from four columns varied widely, as did the observed values. (Measured value of 10.7, 0.1, 0.5 and 1.4 μg/L versus predicted values of 0.0, 0.1, 0.3 and 0.1 μg/L, respectively) PRZM under predicted atrazine concentrations in the upper and lower layers of the soil, but over predicted the concentrations at the middle layers. The authors noted that in three of the four columns studied there was evidence of preferential flow. The authors also conducted a sensitivity analysis and indicated that PRZM was most sensitive to field capacity, bulk density, adsorption coefficients and rate of application.

Trevisan et al. (1993) used the PRZM model (v 1) to examine the leaching of atrazine and metolachlor in a field study in Italy. The model was generally able to predict the experimental data, especially in the top 10 cm. The authors indicated that PRZM underestimated residue levels at 30 cm early in the study, but then agreement was good later in the study. There was no quantitative indication of the actual values so that a better comparison could not be made.

Walker et al. (1995) examined the ability of several models (GLEAMS (runoff only); PRZM (v 2), LEACHP, VARLEACH (leaching only)) to predict the movement of pesticide residues using data from several countries (U.K. (6 locations), Germany (10 locations) France (6 locations), Italy (4 locations)). A wide variety of compounds, including alachlor, chloridazon, metribuzin, metsulfuron-methyl, terbuthylazine were used. PRZM2 tended to over predict, especially at later sampling times, the movement of residues, especially in lysimeter studies. Based on 63 comparisons of the German and French data, PRZM over-estimated the mean leaching depth in 25% of the observations, was within 20% of the measured value in 20% of the observations, and underestimated leaching by more than 20% in 55% of the observations. PRZM over-estimated the residual mass in 25% of the observations, was within 20% of the measured value in 55% of the observations, and underestimated leaching by more than 20% in 25% of the observations. It is interesting to note that there was a wide difference in the ability to predict the values from the French versus the German data sets, as measured by model efficiency, with the French data giving 49% acceptable values while the German data only gave 28% acceptable values. GLEAMS validation efforts were limited to runoff data from one site for 3 seasons and the authors concluded that additional validation and/or modification of the model would be necessary because the model uses input parameters that are related to US measurements, and are not readily available for European situations.

Walker et al. (1996) compared the results of lysimeter studies with alachlor, atrazine and metribuzin to predicted values from PRZM (v 2), VARLEACH and LEACHP. For all three compounds PRZM2 over predicted the movement at later points (112 and 156 days) in the study. Although PRZM under predicted the concentrations of the compounds in the leachate at early sampling events, due to its inability to predict preferential flow, the cumulative losses predicted were within 20% of the measured losses over the length of the study for metribuzin, with no data given for the other compounds.

Zacharias et al. (1994) examined the leaching of bromide, atrazine, and metolachlor over a five month period in a field plot that had been planted to no-till corn in the coastal plain of Virginia using GLEAMS (v 1.8.55) and PRZM (v 2). The modeling used uncalibrated and calibrated simulations. Both the GLEAMS and PRZM models were not able to accurately predict the initial movements of the bromide tracer, with the authors felt was due to both of the models' inability to model preferential flow.

Appendix 2.

FIFRA Environmental Model Validation Task Force (FEMVTF)

Guidance Document For Creating PRZM Input Sequences

Phase II of the Model Validation Project -- Levels I & II*

FEMVTF Input Parameter Subcommittee

Report Date:

June 12, 1998

Revision Number 2.1

* Please note that this document was not used for the generation of Level 1 (cold) simulations but instead a more recent EPA document was used.

I. Scope

This guidance document outlines directions whereby input sequences for PRZM can be created. The model is currently in use by industry, regulatory agencies, and academia. The purpose for this standardization is the hope that as model validation is done, the result will reflect the individual model's ability to perform and not the variability of input sequences. Two levels of validation will be examined. The first level is termed "cold-validation", where no site specific data are used (other than recorded daily weather data) and input data come from standard databases. The objective of Level I is to evaluate how well current regulatory modeling practices fit the observed experimental results. Level I will also determine if longer term simulation runs are required in order to bracket the observed experimental results.

> *Level I Approach:* Use primarily non-site specific data and perform modeling with PRZM3.

The second level of validation will include all available site specific data for use as modeling input. The objective of Level II modeling is to evaluate how well using site specific data the models can predict experimental results.

Level II Approach: Compare site specific data with observed experimental results for the PRZM3 model. One set of chemical inputs (site specific/Registrant) shall be used, as well as, a site specific weather data set.

This guidance document assumes that persons performing model runs are familiar with the various components of the model. In addition to the scope of this document, an EPA guidance procedure is appended to this document and will be run for Level I.

II. Model Version

The model version used shall be the most recently released by the original code generator/distributor. Code modifications from the originally released versions are not allowable for this portion of the work. Currently, for PRZM work version 3.12 shall be used.

III. Development of Input Data Sets

The Task Force (i.e., FIFRA Environmental Model Validation Task Force or FEMVTF) in this document will provide the source of input data necessary to successfully run the model. Again, it is assumed the modeler is familiar with the model and its data input structure. Familiarity includes the ability to convert units as required from the specified data sources.

SUMMARY SHEETS: Summary sheets should be created for each input file, with justification provided for each parameter selected.

BROMIDE TRACE: Be sure the application rate is for a Bromide ion rather than for Potassium Bromide.

FILE LABELING: Meteorological files, input files, and supervisor files should all be labeled in a systematic and unique manner so that the specific site they model can be readily identified. As an example meteorological files, input files, and supervisor files could be named similarly, but differentiated by their file extension. Input files also allow descriptions internally and these should be utilized to further identify which site they model. Information to include, but should not be limited to might be soil series names, phase identifications, and the closest geographical reference, such as Urbana, Illinois. Additionally, each data set will be assigned a reference number for further identification.

The following is offered as an *example* for file identification: SEIL1L01.INP

Contractor Code		**Data Set Code**			**Set Type**	**Run #**			**File Type**		
S	E	I	L	1	L	0	1	.	I	N	P
Stone Environmental		Illinois		Site No. 1	Leaching	1st run			input file		

Contractor Code: SE- Stone Environmental; WB - Waterborne; PE - PTRL-East

Data Set Code: Illinois site 1
Set Type: L - leaching; R - runoff
Run # : 01 1st run
File Type: input

IV. METEOROLOGICAL DATA SETS (LEVELS I & II) *(meteorological data other than site specific is reserved for future work)*

Meteorological data sets should come from the nearest weather station to the site if site specific data are not available. The meteorological data set used should be from the point of collection nearest the actual field site being modeled. If factors such as terrain would preclude the use of the closest site, then the site with the most similar climate to the actual site should be selected. The use of "generic" weather data will provide a reference for the use of probabilistic model runs versus point specific model runs. If on-site weather data sets are not complete, data may be added from the Surface Airways and Summary of the Day CD ROM or other sources at the discretion of the TOC (Technical Oversight Committee). Irrigation will be added to the meteorological file as precipitation. Pan data in each met file will be corrected to an equivalent evapotranspiration rate using *Pan Evaporation x 0.83*.

V. TIME STEP

All model runs should be made in the mode to generate the specified model outputs.

VI. OUTPUT PARAMETERS

A. OUTPUT *LEACHING*

(1) Simulations using site weather data

(a) Annual summary (based on application year)

Year
Annual precipitation (+ snow fall)
Annual recharge (below 1 m or equivalent)
Annual ET
Annual runoff

For chemical and bromide:

Mass of chemical remaining in root zone
Mass of chemical leaching below root zone
Maximum concentration in soil at each soil depth interval
Maximum concentration in soil-pore water at each lysimeter depth

(b) Summaries for monthly field hydrology sampling

Day and Month
Monthly precipitation since 1st application
Monthly recharge since 1st application
Monthly ET since 1st application
Monthly runoff since 1st application

For chemical and bromide:

Monthly cumulative mass remaining in root zone since 1st application at 1 m
Monthly cumulative mass leached below root zone since 1st application at 1 m

(c) Summaries for individual field sampling dates (each parameter conducted for both chemical and bromide separately):

Soil concentration at each sampling depth interval
Soil-pore water at each lysimeter depth

B. OUTPUT *RUNOFF*

(1) Simulations using site weather data (1 year or more)

(a) Annual summary (reserved for future model runs at the discretion of the TOC)

Number of runoff events with detectable chemical in water or sediment
Precipitation between first and last runoff events
Total runoff volume between first and last runoff events
Total sediment yield between first and last runoff events

For chemical :

Total Mass of chemical transported in water phase
Total Mass of chemical transported in sediment phase
Total Mass of chemical transported in water and sediment
Maximum daily chemical concentration in water phase
Maximum daily chemical concentration in sediment phase

(b) Monthly Summaries (reserved for future model runs at the discretion of the TOC)

Month
Number of runoff events with detectable chemical in water or sediment
Total precipitation
Total runoff volume for month
Total sediment yield

For a chemical:

Total Mass of chemical transported in water phase
Total Mass of chemical transported in sediment phase
Total Mass of chemical transported in water and sediment
Maximum chemical concentration in water phase
Maximum chemical concentration in sediment phase

(c) Individual Sampling Event Summaries

Day with runoff event
Precipitation
Total runoff volume
Total sediment yield

For a chemical:

Total Mass of chemical transported in water phase
Total Mass of chemical transported in sediment phase
Total Mass of chemical transported in water and sediment
Maximum chemical concentration in water phase
Maximum chemical concentration in sediment phase

V. MODEL START/STOP DATES AND COMMON INFORMATION

All model runs should begin January 1 of the year the first application is made. The model run duration should be 365 days from the first application or the length of the study, which ever is longer. Weather will be the only variable that changes between each of the model year runs. Additionally, input variables common between models should come from the same database source. Runoff curve numbers, application dates, Kd, for example, should be the same values in each model.

VI. LEVEL I

This Level of Phase II is also referred to as “cold” validation. Model runs here will use no site specific soils data. An attempt to bracket actual field results by using weather in a probabilistic fashion will be undertaken, by running 36 years of meteorological data per site. The Level I validation will provide an estimate of how well current EMWG modeling practices work for generating EECs for ecological and environmental risk assessment. In addition to the above data, the site specific meteorological data should also be added to the file to serve as a “control”. A total of thirty-six years of Athens weather data should be used per run *(reserved for future model runs at the discretion of the TOC).*

A. IRRIGATION

Use of a model’s irrigation simulation routine may be appropriate if the site being modeled was irrigated. If an irrigation technique was used other than sprinkler, the data set should be further examined by Task Force members for its modeling suitability. If the irrigation amounts can not be added as precipitation in the met file, the TOC should be contacted for a decision on how best to further proceed.

B. LEACHING VS. RUNOFF/EROSION

The input parameter selection criterion cited in this document are skewed toward runoff/erosion. However, both the runoff curve number (CN in PRZM) and the universal soil loss cover factor number (USLEC in PRZM) must be minimized to increase infiltration for leaching simulations. Therefore, for the purposes of leaching, set these values to the minimum referenced value.

C. CHEMICAL SPECIFIC PARAMETERS/APPLICATION RATE

Specific chemical properties should be obtained directly from the Registrant or EPA's database. It is required that before chemical parameters are used for modeling that the appropriate sponsor company be contacted for verification that the numbers are accurate. The sponsor company representative should be sent the data set summary sheet prior to modeling for approval. The sponsor company representative working on the task force would be an appropriate contact person. The nominal label rate should be used for this level. Application efficiency shall be 99% (1% spray drift) of the label rate.

D. SOIL PROFILE INFORMATION

Choose all of the following parameters by horizon to a depth of 48" or greater (if the data set indicates) from the Statsgo database. If the Statsgo database value provides a range, use a mean value calculated from the range.

Soil Series Phase -- Select the phase that has all of the available data 1st and 2nd reflects the largest acreage for that soil series

Field Capacity & Permanent Wilt Point -- By horizon go to TABLE 5-25 in the PRZM3 manual; choose a value by texture for your field capacity (FC) value, then subtract the maximum available water content (AWC) value selected from the Statsgo database to determine the permanent wilt point (PWP).

Organic Matter -- Select the mean value cited by horizon for that phase from the Statsgo.

Decay Rates -- EPA methodology will be followed (reserved for future model runs at the discretion of the TOC). The first 48" of the profile should be roughly divided into thirds. The DS rate should equal the DW rate (where DS is the adsorbed phase and DW is the solution phase). The dissipation rate for the first third of the profile should be from the best non-site specific field study. The dissipation rate for the second third of the profile should be the dissipation rate x 2. The dissipation rate for the last third of the profile should be set to the dissipation rate x 3. If the data set requires that soil depths greater that 48" be modeled use the rate x 3 for these depths.

Kd -- Use the best Registrant based values if field data are not available. EPA methodology will be followed *(reserved for future model runs at the discretion of the TOC)*. The Kd value used should be the value that most reflects the modeled soil properties. It is recommended that a multiple regression of Kd verses available soil information can help interpretation. Specific properties to be used in the multiple regression would include such factors as pH, % clay, and CEC. Once a multiple regression of properties has been completed, all soil depths should reflect this selection process.

E. Databases

Chemical specific parameters should come from the EPA's database or from the Registrant.

Soils data should come from the NRCS Statsgo database.

Crop data should come from the USDA Crop Parameter Intelligent Database System (CPIDS) which can be obtained from NSERL at (317) 494-8692.

VII. Level II

Once Level I modeling has been completed, it will be appropriate to begin Level II work. In Level II all of the site specific data available will be used instead of the database values used in Level I. Available soils characterization data will be used, and any other site specific data in that site's database.

A. Irrigation

Irrigation data should be input as precipitation for the years that site specific meteorological data is available.

B. Leaching Vs. Runoff/Erosion

The input parameter selection criterion cited in this document are skewed toward runoff/erosion. However, both the runoff curve number (CN in PRZM) and the universal soil loss cover factor number (USLEC in PRZM) must be minimized to increase infiltration for leaching simulations. Therefore, for the purposes of leaching, set these values to the minimum referenced value.

C. Chemical Specific Parameters

Specific chemical properties should be the best values available from the Registrant.

D. Soil Profile Information

Enter all of the following parameters by horizon to a depth of 48" or greater using all of the site specific data available. If site specific values are unavailable, use the database value that was used from Level I from the Statsgo database.

Soil Series Phase -- use data from the appropriate phase where site specific values are lacking.

Field Capacity & Permanent Wilt Point (PWP) -- use the Rawls & Brackensiek equation with the site specific soil analysis data.*

Application Rate -- Preferred method is to use the time/pass data reported from a study with 1% drift factor.

Organic Matter -- use on-site data.

Compartment Size -- Make compartment sizes as follows:
0.1 cm for 0-10 cm depth
1.0 cm for 10-200 cm depth
2.0 cm for 200-400 cm depth
5.0 cm for >400 cm depth

Decay Rates -- The first 48" of the profile should be roughly divided into thirds. The DS rate should equal the DW rate. The dissipation rate for the first third of the profile should be from the mean field rate from soil dissipation data or the site specific value. The dissipation rate for the second third of the profile should be the rate x 2. The dissipation rate for the last third of the profile should be set to the rate x 3. If the data set requires that soil depths greater that 48" be modeled use the rate x 3 for these depths.

Kd -- Use the best Registrant based values if field data are not available. EPA methodology will be followed *(reserved for future model runs at the discretion of the TOC)*. The Kd value used should be the value that most reflects the modeled soil properties. It is recommended that a multiple regression of Kd verses available soil information can help interpretation. Specific properties to be used in the multiple regression would include such factors as pH, % clay, and CEC. Once a multiple regression of properties has been completed, all soil depths should reflect this selection process.

E. Databases

Use of databases should be minimized for this level of work. However, when it is necessary to use database values, with best expert judgement of the site.

* The task force now recommends the use of site-specific data from undisturbed soil cores when such data is available.

F. Foliar Wash-off/Extraction

Foliar washoff data by compound should be obtained from guideline foliar dislodgeable studies. If site specific foliar washoff information is available, this should be used. The sponsor representative should be contacted to help with this requirement.

G. CN, P, C, and K Factors

For Level II, these values will come directly from the NRCS. Mr. Ken Pfeiffer has agreed to provide the variables by soil series for a specific scenario. In order for Mr. Pfeiffer to provide the proper value, he will need the site specific soil wilt point, field capacity, bulk density (BD), and soil series name. Contact Mr. Pfeiffer at (503) 414-3061.

VIII. Changes to the SOP/Guidance Document

Changes to this Guidance Document can be made by a written, official memorandum from an authorized member of the TOC Committee. Modifications to the SOP/Guidance Document will be made by the TOC Committee.

APPENDIX 1: Toward The Development of Good Modeling Practices in Chemical Fate Modeling

TABLE I. INPUT PARAMETERS FOR PRZM MODEL

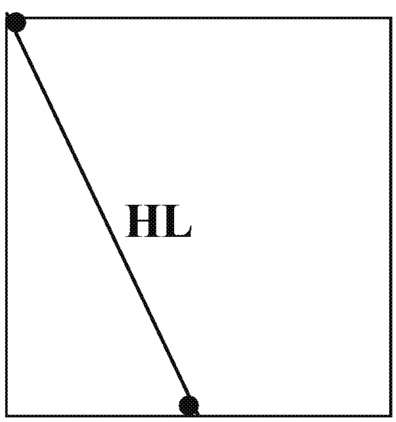
PRZM -- Variable Name	Variable Description	Value	Units	Source
PFAC	Pan factor	Set to 1.0	Dimensionless	PRZM3 manual, Figure 5.1
SFAC	Snow factor		cm melt/C	PRZM3 manual Table 5.1
ANETD	Depth evaporation extracted	10 cm	centimeters	PRZM3 manual , Figure 5.2
ISCOND	Postharvest condition	1	N/A	Or Local Practice - Cooperative Extension
DT	Monthly average daylight	not used	hours	PRZM3 Manual Table 5-2
USLEK	Erodibility factor		dimensionless	NRI (see EPA notes)
USLELS	Slope Length factor		dimensionless	NRI (see EPA notes)
USLEP	Practice factor		dimensionless	PRZM3 Manual Table 5-6 Assume Contour Plowed or Local Practice
AFIELD	Field area	site specific	hectares	Study
CINTCP	crop interception		cm	CPIDS; if no data PRZM3 Manual Table 5-4 (mean value)
AMXDR	Active root depth		cm	CPIDS; if no data PRZM3 Manual Table 5-9
COVMAX	Aerial crop cover	By Crop	percent	CPIDS if no data use PRZM3 default 90%
ICNAH	Post-harvest surface	1	N/A	Standard assumption
CN1	Curve No. - fallow		dimensionless	PRZM3 Manual Table 5-10 to 13 & Statsgo database (hydraulic group)- Average Between Good and Poor
CN2	Curve No. - crop		dimensionless	PRZM3 Manual Table 5-10 to 13 & Statsgo database (hydraulic group)- Average Between Good and Poor
CN3	Curve No. - harvest		dimensionless	PRZM3 Manual Table 5-10 to 13 & Statsgo database (hydraulic group)- Average Between Good and Poor
DSRATE n	Best available Rate		Day-1	DS = DW
DWRATE n	Best available Rate		Day-1	DS = DW
DGRATE n	Vapor decay rate	0	Day^{-1}	Standard assumption
DPN 1	Compartment Thickness	See Text	cm	See Text
THEFC n	Field capacity		cm^3 / cm^3	PRZM3 manual by texture/or Rawls & Brackensiek
THEWP n	Wilting point		cm^3 / cm^3	Statsgo; FC-AWC/ or Rawls & Brackensiek

TABLE I. INPUT PARAMETERS FOR PRZM MODEL, continued

PRZM -- Variable Name	Variable Description	Value	Units	Source
OC n	Organic carbon		percent	Statsgo/site specific
KD n	Partition coefficient		cm^3/gram	Best available regression technology
DPN 2	Compartment Thickness	See Text	cm	See Text
USLEC1	USLE C value fallow		dimensionless	PRZM3 Manual Table 5-7
USLEC2	USLE C value crop		dimensionless	PRZM3 Manual Table 5-7
USLEC3	USLE C value residue		dimensionless	PRZM3 Manual Table 5-7
WFMAX	Crop dry weight		kilo gram/m^2	CPIDS; if no data PRZM3 Manual 5-14
HTMAX	Crop maximum weight		cm	CPIDS; if no data PRZM3 Manual 5-16
EMD, EMM IYREM	Emergence date (day/month/year)		N/A	CPIDS; rationalize with study application date
MAD, MAM IYRMAT	Maturity date (day/month/day)		N/A	CPIDS
HAD, HAM IYRHAR	Harvest date (day/month/day)		N/A	CPIDS
APD, APM IAPYR	Pesticide Application Date (Day/Month/Year)		N/A	From field study
WINDAY	No. moisture checks	0	N/A	not used
DEPI	Incorporated depth		cm	LABEL/PRZM3 Manual 5-15 or from field study
TAPP	Application rate		Kilogram/ha	From field study
APPEFF	Application Efficiency			SDTF values EPA to advise
CAM	Foliar application flag as required		N/A	Label 1-Preplant or Granular 2-Foliar Application
IPSCND	Postharvest deposit	1	N/A	Default; 2 or 3 - Special Conditions
CORED	Depth of soil core	Field Study	cm	From field/analytical data
FEXTRA	Foliar Extraction	0.5	% / cm rain	Default in absence of data /PRZM3 Manual
PLDKRT	Decay Rate On Foliage		Day^{-1}	Registrant
PLVKRT	Plant Volatilization		Day^{-1}	Registrant
UPTKF	Plant uptake factor	1.0	fract of evap	Assumption for FEMVTF
HSWZT	Drainage flag	0	N/A	Assumption for FEMVTF
NHORIZ	Number of horizons		N/A	Statsgo
THKNS n	Thickness horizon		cm	Statsgo
BD n	Bulk density horizon		tones/m^3	Statsgo (high range)

TABLE I. INPUT PARAMETERS FOR PRZM MODEL, continued

PRZM -- Variable Name	Variable Description	Value	Units	Source
THET0 n	Soil water horizon		cm^3/cm^3	THEFC
AD n	Drainage para horizon		liter/day	Determine need from Statsgo
DISP n	Solute Dispersion	0	cm^2/day	Assumption for FEMVTF
DAIR	Diffusion coefficient - Air	0	cm day^{-1}	Assumption for FEMVTF
HENRYK	Henry's Law Constant	0	atm-m^3 $mole^{-1}$	Assumption for FEMVTF
ENPY	Enthalpy of Vaporization	0	cal/mol	Assumption for FEMVTF
KDFLAG	KD/KOC Flag	0	N/A	Not used
PCMC	KD Estimation Flag	0	N/A	Not used
SOL	Solubility	0	mg $liter^{-1}$	Not used
	Mean KOC		liter kg^{-1}	
ERFLAG	Erosion Flag	4		PRZM3 Manual, page 6-26
HL	Hydraulic Length		meters	see below
SLP	Slope		%	Statsgo/field data
IREG	SCS Rainfall Region		N/A	PRZM3 Manual (Figure 5.12)
MNGN	Manning's Roughness Coefficient		dimensionless	PRZM3 Manual (Table 5-46) (value recommended = 0.17)
GDUSLEC	Start *day* of USLEC and Manning's N factors			1 - Simulation Start Day, 2 - Plant Day, 3 - Harvest Day
GMUSLEC	Start *month* of USLEC and Manining's N factors			1 - Simulation Start Month, 2 - Plant Month, 3 - Harvest Month



Assume square field, calculate HL

APPENDIX 1:

Toward the Development of Good Modeling Practices in Chemical Fate Modeling

TOWARD THE DEVELOPMENT OF GOOD MODELING PRACTICES IN CHEMICAL FATE MODELING

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Abstract

Applications of chemical fate modeling are becoming increasingly important in the pesticide registration process. It is therefore necessary to identify "Good Modeling Practices" (GMPS) to insure that credible results are derived using certified models. The EPA and National Agricultural Chemical Association (NACA) have jointly formed a working group to address this and many other issues of chemical fate modeling as it relates to pesticide testing and registration. This paper will introduce the working group's current thoughts and recommendations for GMPS. Included will be model development issues related to the testing, documentation, distribution and maintenance of source codes. Issues relating to model users include the selection of suitable models, identification and documentation of input data, addressing uncertainty in model input parameters and adoption of suitable test scenarios to meet scientific and regulatory needs. The need to adopt somewhat standardized methods of reporting will also be addressed.

Introduction

Chemical environmental fate models have become widespread tools for assessing the fate of pesticides in the environment. Use of such models is now becoming an integral part of the pesticide registration process. Results from environmental fate models are used to assess pesticide behavior in the soil, ground water, runoff, surface water and air.

To address some of the concerns about model usage in the testing and pesticide registration process, the U.S. Environmental Protection Agency (EPA) and the National Agricultural Chemical Association (NACA) have jointly formed the Exposure Modeling Work Group (EMWG). This group is comprised of some twenty participants representing the agricultural chemical industry, EPA, government agencies and scientific consultants.

A concern of the EMWG is that with the increase in demand for environmental assessments, it is critical that the integrity of the model development, maintenance and usage be assured. For this reason, it is necessary to identify "Good Modeling Practices" (GMPS) to assure the quality of the modeling effort. This paper will discuss the FIFRA EMWG current thoughts and recommendations for GMPS.

Discussion

In this paper, "Good Modeling Practices" is defined as the development, maintenance, distribution and use of computer simulation models whereby the integrity of the model, its various improvements and utilization is assured. GMPs should be followed during every step of the modeling process, from model development to model usage by the scientific community. Individuals involved in GMPs have been grouped into three categories: the model developer, the model maintainer and the model user. Each category has its own set of responsibilities for maintaining GMPs in chemical environmental fate modeling.

Responsibilities of the Model Developer

The category of model developer includes any individual who is the actual creator of a model. Given the complexity of current environmental fate models, it is recognized that development teams are often required to produce a model. These development teams also belong to the category of model developer.

The model developer is responsible for model conceptualization. The purpose and appropriate uses of the model should be dearly defined early in the development process. Once the conceptual model is designed, the model developer is responsible for the assimilation of the appropriate mathematical algorithms and then development of the computer source code. The model developer should identify significant assumptions and limitations of the model. After the model is developed, the model developer is responsible for testing the model to assure that it performs as designed. Testing should involve computer source code debugging and confirmation that the mathematical algorithms are generating expected results. The model developer may choose to have the model "beta" tested by other scientists in the modeling community. The model developer is responsible for validating the model results against a reasonable collection of "real-world" data to assure that results from the model are realistic. Validation helps identify assumptions and limitations of the model as well as quantifying the uncertainty associated with use of the model. Any necessary refinements should be made. Once refined, the model should be tested and validated again. Results from the testing and validation exercises should be documented allowing for future examination of the strengths and weaknesses of the model.

The model developer should be responsible for generating a series of test files to be issued with the model. These test files should include both model input files and their associated expected output files. The purpose of the test files is to enable users to confirm that the model is working correctly on computer systems other than the one on which it was developed.

Documentation is very important during every step of the model development process. Documentation should be dear and sufficiently detailed so that the model can be used and maintained by individuals other than the developer. Documentation should include discussion of the theoretical model, computer systems support information, instructions on how to use the model and any other information necessary to assure correct use of the model. If the model is revised, the documentation should be updated reflecting the changes. The model developer is responsible for producing and revising the model documentation.

<u>Responsibilities of the Model Maintainer</u>

The category of model maintainer includes any individual who is responsible for the model once it has been issued for public use. The model developer may perform this maintenance role or this function may be given to an independent source. The model maintainer should be designated as the keeper of the "official" source code for both the current and previous versions of the model. The model maintainer serves as an information and communication source for the user community. He/she is responsible for maintaining and distributing the model, associated documentation, related databases and input/output test files. This individual is also responsible for tracking model version changes and notifying the user community about model upgrades. Version tracking includes communication with the user community about which versions of a model are considered acceptable for use. As models are enhanced, previous versions may be deemed unacceptable due to improvements in algorithms or correction of software bugs.

As part of the communication responsibility, the model maintainer should keep an error log of software and algorithm bugs reported by users. These bugs should be reported to the model developer. The model developer should communicate information about model upgrades to the model maintainer. The model maintainer may assist in documenting any modifications or enhancements made by the model developer.

A major responsibility of the model maintainer is to be a source of education about the model for the user community. This education can be provided in many different ways. Education is provided by distributing and maintaining the user's manuals. Technical support to the users is another form of education about the model. Availability of technical support may be in the form of telephone support lines, computer on-line help systems, written communication or workshops. All of this educational support is the responsibility of the model maintainer.

<u>Responsibilities of the Model User</u>

The category of model user includes any individual who uses the model to generate predictive results for assessing the fate of pesticides in the environment. For the model user, GMPs are concerned with the correct use of the model, proper interpretation of model results, and adequate documentation of the modeling work. The goal is to assure the quality of the modeling effort.

The model user is responsible for understanding the model and its appropriate usage. This includes understanding the assumptions and limitations of the model. The assumptions should be examined with each new study to assure that the scenario being examined does not violate any of the model assumptions. The scenario should also be examined to confirm that it is within the acceptable limitations of the model. The model user should avoid viewing the model as simply a "black-box" into which input-information is fed and results are mysteriously produced thereafter.

When modeling, the model user should develop simulation scenarios that match their intended goals. The model user should chose geographical areas, weather information, chemical properties and environmental conditions that adequately represent the scenario being simulated. Input data should be carefully examined to confirm that it is correct. This avoids the "garbage in, garbage out" problem. Special attention should be paid to assure that the input information is in the correct units required by the model. When input information is unavailable and needs to be estimated, care should be taken to evaluate the uncertainty of the estimate. This may involve simulating the variable over a range of values for the uncertain input parameter. Uncertainty is especially important for weather data. Due to the variability in weather conditions, 20 to 30 years of weather data is more representative of the weather pattern at a geographical site than the selection of a single weather year.

Model output must be examined to confirm that the results are reasonable. Unjustified extrapolation of model results must be eliminated. Results from a single geographical site should not be extrapolated to other locations with environmental conditions different from the simulated site.

The model user should stay current with accepted versions of the model and stay current with the documentation. Additionally, this individual is responsible for assuring computer source code integrity. A copy of the original source code should be maintained by users inclined to make changes. Any changes to the source code should be documented in the modeling report. Modified versions of the source code must be clearly identified to maintain the model integrity in the public domain.

The user is responsible for developing modeling reports which contain sufficient information for an independent source to reproduce the same results. The report should identify both the model and version used. If the model was modified, a copy of the modified source code should be included with the report. Input information needs to adequately discussed. Representative copies of the input data files should be attached.

Conclusion

Simulation modeling is a useful methodology for chemical environmental fate modeling and is expected to become an increasingly important part of the environmental assessment process. With the expected increase in model usage, it is critical that the integrity of the model development, maintenance and use be assured. All individuals who develop, distribute, use **or** interpret models or modeling results have **a** responsibility to follow GMPs to assure the quality of the modeling effort.

References

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Dougherty, D.E. and A.C. Bagtzoglou. 1993.. A Caution on the Regulatory Use of Numerical Solute Transport Models, *Ground Water 31:1007-1010*.

Gorlitz, G. 1993. Rules for the Correct Performance and Evaluation of Model Calculations for Simulation of the Environmental Behaviour of Pesticides.Biologische Bundesanstalt fur Land- und Forstwirtschaft, Fraunhofer Institut fur Umweltchemie und Okotoxikologie, Arbeitsgruppe "Simuladonsmodelle" im Industrieverband Agrar (IVA), Umweltbundesamt.

Appendix 3. Guidance for the Performance of Calibrated Modeling

The third level of modeling to be performed for the FIFRA Exposure Model Validation Task Force (FEMVTF) is calibrated modeling and is designated as Level 2A modeling. For this modeling work, the modeler is provided with both the necessary input data from the field study (e.g. the weather data, soil data, chemical data and agronomic data) as well as the experimental results (e.g. concentrations of chemical and tracer in soil and water over time) and necessary supporting experimental data (study records).

With the availability of the experimental results, it is possible to refine (or calibrate) the values of selected model inputs to provide closer agreement between model predictions and observed field data.

The purpose of model calibration is threefold:

(1) To determine which parameters require adjustment from the more general values that were used in cold and site-specific modeling

(2) To determine the improvement in fit between model predictions and experimental data

(3) To identify model algorithms/components and field data values which may require improvement to increase the future accuracy of both models and field studies

It should be clearly recognized that both the observed field results and the predicted modeling results contain error. Neither value should be regarded as absolutely correct. Field data incorporate the cumulative errors from uneven application; sampling error; handling, processing and storage effects; and analytical error. Additionally, field data may be limited with respect to data density that restricts both the spatial/temporal scales of data resolution and the types of data taken. Modeling results include errors from violation of assumptions; idealistic treatment of complex environmental behavior; and mathematical errors due to spatial, temporal or numerical problems.

The general guidance for calibrating modeling to experimental results is to first calibrate the hydrology of the model to provide a reasonable representation of water movement at the specific study site. In the case of runoff modeling, calibration of erosive sediment loss is an important secondary consideration. Once these steps are done, then the simulation of the transport and dissipation of the chemical can be evaluated and calibrated, as necessary. Calibration of chemical transport and dissipation should consider the phase distribution for the chemical. For example, for a highly sorbed molecule chemical calibration should first consider the chemical in the soil/sediment phase and then the chemical in the water phase.

For the purposes of the FEMVTF project, model input parameters should be adjusted based on study specific information or sensitivity analysis that justifies the change. For instance, study observations of soil sealing due to in-crop rainfall events may suggest a change in curve number as a step in calibration to better fit late season hydrologic events. Adjustments should not be made outside of the ranges that are reasonable. If parameter adjustment beyond a reasonable range is required to achieve a satisfactory fit, then there is potentially a problem either with the model or the experimental data. Using unreasonable input values is an unacceptable method to achieve improved modeling results.

Guidance for Calibration of Leaching Modeling

Hydrologic Calibration

The movement of water in a typical prospective ground water study is not directly measured. Depending upon the field study, there are various types of climatic and hydrologic data available:

- Daily precipitation
- Daily irrigation data
- Daily evapotranspiration (usually calculated)
- Daily runoff
- Daily soil moisture at various depths
- Periodic measurements of bromide ion in soil, soil pore water and ground water

The daily precipitation and irrigation data are provided in the input weather file for each study site. If the weather data were obtained from an on-site weather station, they should be regarded as fixed data. If the weather data were obtained from a regional weather station, then the reported daily values are potentially adjustable if no other adjustments provide adequate fit to the experimental results. Ideally, irrigation data should be measured at multiple locations and averaged. Since this is rarely done, experimental irrigation data should be regarded as subject to measurement error, especially irrigation using method prone to uneven distribution such as travelling guns or flood irrigation. The study records should be consulted to determine the accuracy of irrigation events.

For FEMVTF modeling, evapotranspiration data is calculated external to the model and is provided as an input to the model via the weather file. Calculated ET values are approximate and can be adjusted if necessary to obtain an improved water balance. Adjustments can be made either directly to the weather file or via the pan factor.

Runoff is usually negligible at the sites where ground water studies are conducted. However, this should be confirmed from the study records.

The infiltration of water is not directly measured in ground water studies. Instead, measurements of soil moisture and tracer fate are available which allow estimation of the amount of recharge that occurred at the study site. Soil moisture conditions at various depth intervals above the root zone provide a general indication of when recharge events occurred.

The most useful data for calibration of infiltration is bromide data. Bromide data in soil, soil pore water and ground water can provide at least three types of information:

- Information on the movement of water due to normal matrix flow through the soil profile (i.e. the movement of the center of mass of bromide)
- Information on the extent of preferential flow events relatively soon after application
- Information on the extent of dispersion (band broadening) during infiltration

For model validation, the most valuable information is the use of bromide to estimate the time required for water to move to a specific depth in the soil. Bromide is used as a tracer in ground water studies because it is conservative (not degraded in soil) and it is essentially unadsorbed in the soil profile. It should be recognized that most actively growing crops take up bromide and overall recoveries of 40-80% of applied bromide are typical. Due to the loss of bromide via root uptake, it is best to characterize the rate of movement of bromide from depths below the root zone (typically three feet or more).

The movement of bromide below the root zone should be estimated from the approximate center of mass in the soil profile. If the distribution of bromide in the soil profile is somewhat symmetrical, this corresponds to the location of the peak concentration. The movement of the center of mass of bromide as simulated by the model should correspond to that observed in the field experiment. Both the model and the field data should approximately correspond with published estimates of typical recharge rates for a specific site.

The first detection of bromide in suction lysimeters and wells can provide a valuable insight into whether the study site has a significant amount of preferential flow. Bromide observed in lysimeters or wells significantly in advance of the leading edge of bromide simulated by the model may indicate that the model is not representing this movement. This may be due to the model lacking a preferential flow component or due to inappropriate specification of the dispersion coefficient in the model.

In cold and site-specific modeling, the dispersion coefficient is set to 0.0 and dispersion is implicitly determined by the selected spatial compartment size. In an effort to improve the accuracy of runoff and leaching calculations, the FEMVTF has specified that 0.1 cm compartments be used in the top 10 cm of the soil profile and 1 cm compartments used at deeper depths. One result of using these compartment sizes is the simulation of less dispersion in the soil profile than would result from the use of 5-cm compartments (the recommendation in the PRZM manual to allow numerical dispersion to mimic physical dispersion). If significant initial detections of bromide are observed but not simulated by the model, the effect of compartment size should be evaluated and/or additional dispersion should be added using the parameter DISP. If the initial bromide detections cannot be simulated using either 5-cm compartments or the addition of reasonable amounts of added dispersion, then it must be concluded that some degree of preferential flow occurred at the study site.

To complete the hydrologic calibration, an annual mass balance should be constructed for the study site summarizing the water inputs (precipitation and irrigation) and water outputs (evapotranspiration, plant uptake, runoff and leaching). The percent annual recharge to a depth below the root zone (e.g. 1 m) from the date of chemical application should be explicitly calculated.

Chemical Calibration

Depending upon the chemical use patterns, there are a number of parameters that may require calibration to match the results from a specific field study:

- For all pesticides, the following application parameters should be modified to fit the measured field data, considering the following data:
  - actual rate of application (versus nominal)
  - extent of canopy interception (if any)
  - actual rate of soil interception (from filter discs or equivalent)

- For foliarly applied pesticides, the following parameters are important and should be modified to fit available field data:
  - rate of degradation/volatilization from the crop canopy
  - rate of washoff via rainfall and irrigation

- To modify the rate of movement, Kd should be adjusted within the range of the available experimental data for the chemical and soil properties in the various soil horizons

- To modify the rate of degradation, the chemical half-life in the soil should be adjusted with depth (and time, if necessary and appropriate) in accordance with available information on the degradation behavior of the chemical. Particular attention should be given to assessing the most appropriate values of chemical half-life with soil depth since this relationship is generally based on assumptions rather than measured data. For chemicals that degrade slowly, it may be appropriate to consider seasonal variation in the half-life to reflect the effects of environmental temperature variations.

Guidance for Calibration of Runoff Modeling

Hydrologic Calibration

Runoff events are generally directly measured in field runoff studies. The timing and volume of individual runoff events are available for comparison with modeling results. To calibrate a runoff model to a field study, it is important to consider the accuracy of the various experimental parameters that affect the experimental data and predicted results:

- Daily precipitation and irrigation events during the period when runoff events occur
- Daily evapotranspiration
- Daily runoff
- The treated area which is drained to the point where runoff is measured
- The selection of curve number (based on crop, management practice, soil type and hydrologic condition)
- Soil parameters influencing runoff and erosion (e.g. field capacity, wilt point, bulk density and organic matter content)
- Universal soil loss equation parameters (USELK, USLELS, USLEP, USLEC) and the experimental parameters which determine these values

Experimental runoff data is generally provided in units of volume/time where modeling runoff values are typically reported in units of depth/time. The treated area that produces the runoff is therefore a key parameter in calibrating experimental results to modeling predictions.

Runoff studies measure surface losses of water on an event basis and may contain data on water storage (soil moisture with depth) and estimated evapotranspiration. Runoff studies rarely have experimental data that allow parallel evaluation of the extent of infiltration at the study site. Therefore, calibration of the hydrology for a runoff study consists primarily of matching the observed runoff events with the predictions of the model. Comparison of measured runoff yields and total incident rainfall plus irrigation to the model hydrologic summary can be used for calibration to the observed hydrologic routing. The primary factors influencing the observed volume of runoff will be the curve numbers and the antecedent soil moisture condition. Curve numbers can frequently be directly calculated from the reported results of the field study. In some instances, runoff data for conservative tracers of water movement (bromide or early events for the application of a weakly sorbed pesticide) may be used to determine if the model simulation of site hydrology is appropriate.

The use of daily time steps to simulate runoff may not afford sufficient resolution to simulate site events. Observed rainfall events of greater than one-day duration may justify repartitioning of rainfall distribution among the days of the event to better simulate the timing and intensity of events.

To complete the hydrologic calibration of runoff, a mass balance for the study duration should be constructed for the study site summarizing the water inputs (precipitation and irrigation), water outputs (evapotranspiration, runoff and leaching) and erosive soil losses. The percent runoff and soil losses should be explicitly calculated for the time between application and the last reported runoff event. Runoff and erosion values should be compared to other available literature to ensure that the results are reasonable.

Chemical Calibration

Depending upon the chemical use patterns, there are a number of parameters that may require calibration to match the results from a specific field study:

- For all pesticides, the following application parameters should be modified to fit the measured field data, considering the following data:
  - actual rate of application (versus nominal)
  - extent of canopy interception (if any)
  - actual rate of soil interception (from filter discs or equivalent)

- For foliarly applied pesticides, the following parameters are important and should be modified to fit available field data:
  - rate of degradation/volatilization from the crop canopy
  - rate of washoff via rainfall and irrigation

- To modify the rate of movement, Kd should be adjusted within the range of the available experimental data for the chemical and soil properties in the surface horizon.

- To modify the rate of degradation, the chemical half-life in the soil should be adjusted in the top soil horizon. Obviously, degradation rates at deeper soil depths do not impact the observed runoff results.

Appendix 4

FIFRA Environmental Model Validation Task Force

Phase II of the Model Validation Project — Level I & II

Guidance Document

for

PRZM Sensitivity Analysis

Using PB Version 1.2

18 September, 1998

Guidance Document for PRZM/GLEAMS Sensitivity Analysis Using PB Version 1.2

I — Scope

This FIFRA Environmental Model Validation Task Force guidance document outlines methodology for evaluating PRZM output for sensitivity to variation in input data. The objectives of this sensitivity analysis are to

(1) "Validate" expert model user opinion as to the critical input data requirements for leaching and runoff modeling by PRZM.

(2) Identify and rank the sensitivity of key input data for each specific data set evaluated in the FEMVTF Phase II exercise.

The results of the sensitivity analysis will provide quantitative information as to the overall acceptability of the input data set and criteria for creating input parameter combinations.[1] These results will allow for more comprehensive interpretation of results for the Level 1 and Level 2 model validation exercises.[2]

II — Model Versions, Input Datasets, and Development of Model Input Sequences:
The sensitivity analysis will utilize methodology described in the "Guidance Document for Creating PRZM Input Sequences."[1]

III — Sensitivity Analysis Program

The FEMVTF has selected the Plackett-Burman (PB) design approach for evaluation of sensitive inputs for PRZM (Appendix A). The sensitivity analysis program has three components:

(1) A FORTRAN program for the sensitivity analysis using a PB design that generates model input files.

(2) A shell script (batch file) that executes the PRZM3 model and FORTRAN statistical summary programs.

(3) Summarization of statistical results for input and output parameters investigated.

The sensitivity analysis program can be obtained from FEMVTF; PRZM may need to be recompiled for a specific hardware platform once the output format subroutine has been incorporated. Version 1.2 of PB is to be employed using PRZM3 version 3.12 beta from CEAM (ftp://ftp.epa.gov/epa_ceam/wwwhtml/softwdos.htm).

IV — Conducting the Sensitivity Analysis

The input parameter combinations are first created for each dataset according to the relevant guideline document.[1] The PB Readme.txt file should be consulted for specific information on installation and use of the model version being employed.

(1) **General**. Individual sensitivity analyses are to be conducted for each model output parameter of interest as follows:

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[1] Lin, J., S. Jackson, R. Jones, R. Parker, M. Russell. 1998. Guidance Document for Creating PRZM Input Sequences. Revision 2.1. 12 Jun 98. FIFRA Environmental Model Validation Task Force.
[2] Level 1: "Cold validation" where, other than daily recorded weather data, input data comes exclusively from standard databases. Level 2: Comprehensive site-specific input data are used.

Runoff via PRZM:
Total Runoff Flux (mg/ha/year)
Total Erosion Flux (mg/ha/year)

Leaching via PRZM:
Maximum Total Pesticide In Compartment X (mg/kg)[3]
Maximum Pesticide Dissolved In Compartment X (mg/L)
Total Dispersion Flux At Soil Core Depth (mg/ha/year)

step 1: If using PRZM for runoff, set STEP1=STEP2=STEP3=YEAR in the Przm.in file. If using PRZM for leaching, set STEP1=STEP2=YEAR and STEP3=DAY in the Przm.in file.

step 2: Select a compartment depth at the midpoint of the second soil layer specified in the input file.

Two analyses will be conducted for each dataset-model combination using the best available site-specific data (Level 2 modeling): quasi-global and constrained. General rules for preparing the source data (a PRZM3 ver. 3.12 input file) for analysis are as follows:

Inspect the source PRZM input file for the sensitivity and identify those inputs that when adjusted by the perturbation factor (PF) will exceed acceptable input limits for PRZM. For these inputs either adjust the input so that when perturbed bounding limits will not be exceeded (preferred approach), or eliminate this parameter from consideration by PB (that is, do not perturb).

Do not perturb input parameters that are set to zero (0) in the source file.

Truncate the source met file to include only 1 year of data.

Monitor the outp.dat file created by PB to determine if PB-generated PRZM runs are properly executing. Note in particular that if total dispersion flux is showing fluxes well below the method sensitivity for the pesticides being modeled that the soil core depth should be adjusted upward through modification of the source input file (selection of a soil core depth within the described root zone at less than 100 cm is preferred).

Refer to the documentation for PB version 1.2 for further details regarding execution of PB runs.

(2) **Quasi-global analysis.** This analysis considers all input parameters implemented within the PB program for a given model (a maximum of 64 possible inputs for PRZM, Appendix B). This portion of the sensitivity analysis serves as a check on dataset quality parameters used as the basis for dataset inclusion into the FEMVTF exercise.

step 1: When prompted by the PB program "What percentage around nominal values would you like to perturb?" enter **0.10** as the perturbation factor (PF) — this will cause the PB program to vary the inputs selected for analysis by ±10% of the nominal value for the dataset.

step 2: Perform sequential runs where PF is lowered from 0.10 in steps of 0.02 to the point where the range in output probability of a greater |T| (Pr > |T|) ranges from zero (0.0000) to approximately 1 for the output correlation of interest. This is the optimized PF.

(3) **Constrained analysis.**

step 1: Exclude those parameters identified as not sensitive (Pr |T| ≥ 0.05) from the quasi-global analysis at the optimized PF.

step 2: Rerun PB at the optimzed PF for this reduced set of inputs.

V — Reporting the Results of the Sensitivity Analysis

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[3] Where "X" is the layer of interest input by the modeler. This may represent the lowest computational layer at which a detect occurs or the computational layer where the center of mass occurs.

Sensitivity analysis will be completed in conjunction with Level 2 modeling. Relative sensitivities for a given PB model run are calculated as E/E_{max}, where E is the effect for an input parameter and E_{max} is the maximum effect observed for the parameters input into the PB run. Results of the quasi-global analysis are plotted as E/E_{max} versus parameter number (Appendix B). Results of the constrained analysis, expressed as $|E/E_{max}|$, are plotted as a pie chart. Output examples are found in Appendix C.

Appendix A: Overview of Plackett-Burman Analysis

PB analysis affords a simple approach for the identification and ranking of variance components in multiparametric models.[4] Identification of the limited "primary" variables controlling model outcomes allows for stepwise refinement of the model through identification and control of the "primary" variables. PB analysis isolates the main effect of a variable in a model through a contrast of outcomes at two different levels of the variable. This is accomplished by investigating equal numbers of combinations of each variable at predetermined "high" and "low" levels dictated by the selection of the perturbation factor. The average difference in outcomes over the various combinations of variable input parameters allows for determining the effect of change per unit for each input parameter. Inclusion of a subset of dummy variables produces a model error component that can be used to test the variance of each input parameter of the model.

PB design uses an incomplete block factorial design where each input parameter is evenly weighted. This reduces the number of unique model simulations required at the expense of assuming that interactions between more than two variables are insignificant, as this variance is grouped with the model error. Designs for contrasts at two levels are presented by Plackett and Burman (1946).[4]

Analysis of the results of a PB design is straightforward. First, the average difference in the sum of "high" and "low" inputs for the test and dummy parameters is determined. The standard error variance of an effect (V) is the variance due to dummy variables (E_{Di}, where i = 1,n with n being the total number of dummy variables; typically, n = 5 degrees of freedom for the PB program):

$$V = \frac{\sum_{i=1}^{n}\left(E_{D_i}\right)^2}{n}$$

The standard deviation of the effect is thus,

$$s = V^{1/2}$$

A simple t-test allows for testing of the significance of the effects found for the mean difference between two real variables (X):

$$t = (X_h - X_l)/s_x$$

$$\text{where } s_x = \frac{s}{\sqrt{n}}$$

The result of PB analysis is, therefore, a ranked listing of variables in order of their relative effect on model outcomes along with a determination of relative significance of the effect. PB analysis has been used to evaluate input parameter sensitivity for transport modeling of pesticides at the regional scale.[5,6,7]

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[4] Plackett, R. L. and J. P. Burman. 1946. The design of optimum multifactorial experiments. *Biometrika* 33:305-325.

[5] Cryer, S. A., P. L. Havens, R. A. Swearington, and P. G. Nordstrom. 1994. Addressing regional runoff variability using a binned interval approach. 748 *In* Abstr. 8th Intern. Congr. Pest. Chem., 4—9 Jul, 1994, Washington, D. C.

Soil Correlations To Eliminate Potential Nonsense Parameter Combinations.[8]

In addition to the experimental design considerations, several physically based correlations for soil properties are employed to avoid possible "nonsense" parameter combinations that can be obtained from the PB analysis. The following simple equality must be obeyed for all soils.

$$\text{Wilting Point (WP)} \leq \text{Field Capacity (FC)} \leq \text{Porosity (POR)} \qquad \{1\}$$

It is possible that if WP, FC, and POR are treated as independent parameters with certain magnitudes, that the PB design could dictate that the equality of equation 1 does not hold. This typically causes the GLEAMS model to generate erroneous results or not run at all. Soil correlations in the PRZM model are implemented for both the GLEAMS and PRZM models to avoid potential nonsense soil parameter combinations.

$$FC(i)= 0.3486 - 0.0018\ SAND(i)+ 0.0039\ CLAY(i) + 0.0228\ OM(i) - 0.0738\ BD(i) \qquad \{2\}$$

$$WP(i) = 0.0854 - 0.0004\ SAND(i) + 0.0044\ CLAY(i) + 0.0122\ OM(i) - 0.0182\ BD(i) \qquad \{3\}$$

$$BD(i) = 2.65\ [1 - POR(i)] \qquad \{4\}$$

The array subscripts "(i)" in equations **{2}** or **{3}** represent layers i, from i = 1 to i = total number of soil layers that are being modeled.

In these correlations, both WP and FC are treated as dependent variables and are functions of soil texture (% CLAY and % SAND), bulk density (BD) , and soil organic matter (OM). Thus, % SAND, % CLAY, OM and BD can be investigated in the sensitivity analysis. FC and WP are calculated from these independent variables. Certain parameter combinations substituted into equations **{2}** — **{4}** do not satisfy equation **{1}** In cases where WP > FC, WP is set equal to FC minus a small amount. In cases where FC > PRO, FC is set to a value slightly less than POR. This guarantees that equation **{1}** would always hold true for all independent variable combinations regardless if the parameter combinations were real or imaginary.

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[6] Fontaine, D. D., P. L. Havens, G. E. Blau, and P. M. Tillotson. 1992. The role of sensitivity analysis in groundwater risk modeling for pesticides. *Weed Technol.* 6:716-724.
[7] Cryer, S. A., and P. L. Havens. 1997. Regional sensitivity analysis for the USDA model GLEAMS. J. Environ. Qual. (submitted).
[8] Exerpted from Cryer, S. A. 1996. Plackett and Burman experimental design sensitivity analysis for the environmental fate models GLEAMS, SWRRBWQ, EPICWQ, and PRZM-2. Manuscript in draft.

Soil properties which vary with depth. Several soil properties can vary with depth throughout the soil horizon. Examples include porosity/bulk density, field capacity, wilting point, organic matter, and pH. The user specifies as input the soil depth increments where property values differ, along with the magnitudes of the properties at each specified depth. The number of PB simulations required if all soil intervals were modeled as being independent would dramatically increase if each soil layer were treated as a separate entity. Therefore, parameters that can change with depth are grouped together and changed according to the original user defined magnitude (via the nominal file) at each depth. For example, if soil organic matter is chosen as an input parameter to investigate, the PB program changes all soil organic matter by the same perturbation factor specified by the user. If the user specifies a 10 percent perturbation around the nominal value and the PB design specifies a "-1", then all of the soil organic matters values for each soil layer and for this simulation are decreased by approximately 10 percent. Thus, the same value for organic matter is not simulated for all soil depth intervals, (unless the user specifies the organic matter does not vary with depth in the nominal file) but rather a consistent and constant percent change occurs for each depth value.

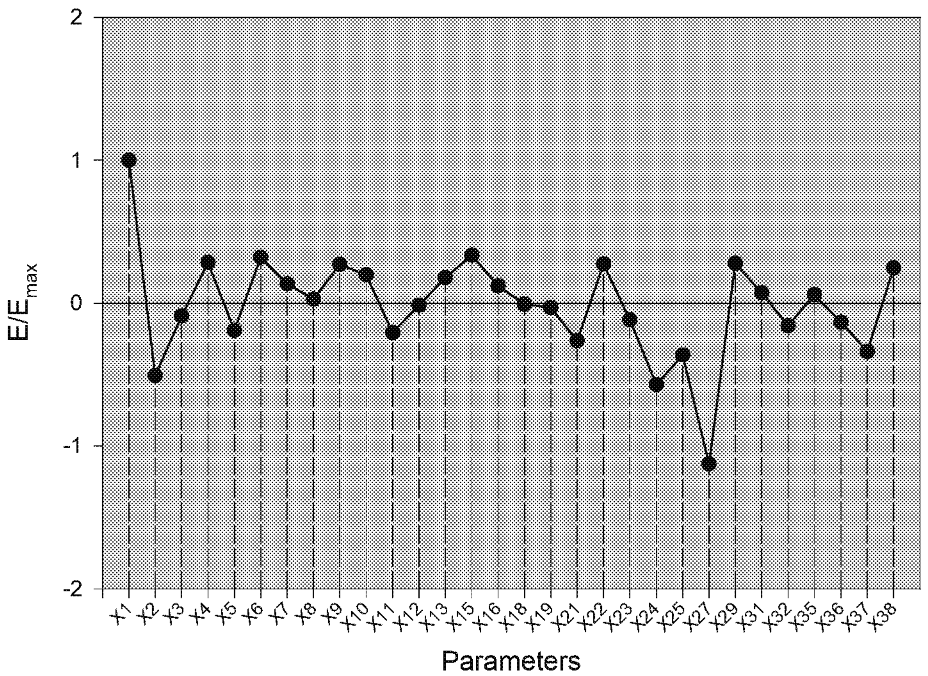
Appendix B: PRZM3 Model Input Parameters Implemented by PB

```
 1) PAN FACTOR
 2) MIN DEPTH WHICH EVAP. IS EXTRACTED
 3) MAX INTERCEPT STORAGE OF CROP
 4) MAX ROOTING DEPTH OF CROP
 5) MAX AREAL COVERAGE OF CANOPY
 6) R.O. CURVE # 1 OF ANTE MOIST COND II
 7) R.O. CURVE # 2 OF ANTE MOIST COND II
 8) R.O. CURVE # 3 OF ANTE MOIST COND II
 9) UNI SOIL LOSS COVER MGT FACTORS
10) MANNINGS N
11) HYDROLIC LENGTH
12) SLOPE (SLP)
13) MAX DRY WGT OF CROP FULL CANOPY
14) MAX CANOPY HEIGHT
15) DEPTH OF PESTICIDE APPLICATION
16) TOTAL APPLICATION OF PESTICIDE
17) FILTRATION PARAMETER
18) PEST. VOLATIL. DECAY RATE ON FOLIAGE
19) PESTICIDE DECAY RATE ON FOLIAGE
20) FOLIAR EXTRACT. COEFF FOR PLANT W.O.
21) PLANT UPTAKE FACTOR
22) DIFFUSION COEFF FOR PEST IN AIR
23) HENRYs LAW CONSTANT
24) ENTHALPY OF VAPORIZATION
25) PESTICIDE SOLUBILITY
26) BULK DENSITY/MINERAL DENSITY
27) INITIAL SOIL WATER CONTENT OF HORIZON
28) SOIL DRAINAGE PARAMETER
29) PEST SOLUTE DISP. COEFF.
30) VAPOR PHASE PESTICIDE DECAY RATE
31) THICKNESS OF HORIZON COMPARTMENT
32) % SAND
33) % CLAY
34) HORIZON ORGANIC CARBON
35) DISSOLVED PHASE DECAY RATE (1)
36) ADSORBED PHASE DECAY RATE(1)
37) PESTICIDE PARTITION COEFFICIENT(1)
38) DISSOLVED PHASE DECAY RATE (2)
39) ADSORBED PHASE DECAY RATE(2)
40) PESTICIDE PARTITION COEFFICIENT(2)
41) DISSOLVED PHASE DECAY RATE (3)
42) ADSORBED PHASE DECAY RATE(3)
43) PESTICIDE PARTITION COEFFICIENT(3)
44) DISSOLVED PHASE DECAY RATE (4)
45) ADSORBED PHASE DECAY RATE(4)
46) PESTICIDE PARTITION COEFFICIENT(4)
47) DISSOLVED PHASE DECAY RATE (5)
48) ADSORBED PHASE DECAY RATE(5)
49) PESTICIDE PARTITION COEFFICIENT(5)
50) DISSOLVED PHASE DECAY RATE (6)
51) ADSORBED PHASE DECAY RATE(6)
52) PESTICIDE PARTITION COEFFICIENT(6)
53) DISSOLVED PHASE DECAY RATE (7)
54) ADSORBED PHASE DECAY RATE(7)
55) PESTICIDE PARTITION COEFFICIENT(7)
56) DISSOLVED PHASE DECAY RATE (8)
57) ADSORBED PHASE DECAY RATE(8)
58) PESTICIDE PARTITION COEFFICIENT(8)
59) DISSOLVED PHASE DECAY RATE (9)
60) ADSORBED PHASE DECAY RATE(9)
61) PESTICIDE PARTITION COEFFICIENT(9)
62) DISSOLVED PHASE DECAY RATE (10)
63) ADSORBED PHASE DECAY RATE(10)
64) PESTICIDE PARTITION COEFFICIENT(10)
```

Appendix C: Example summarization of model sensitivity for PB output.

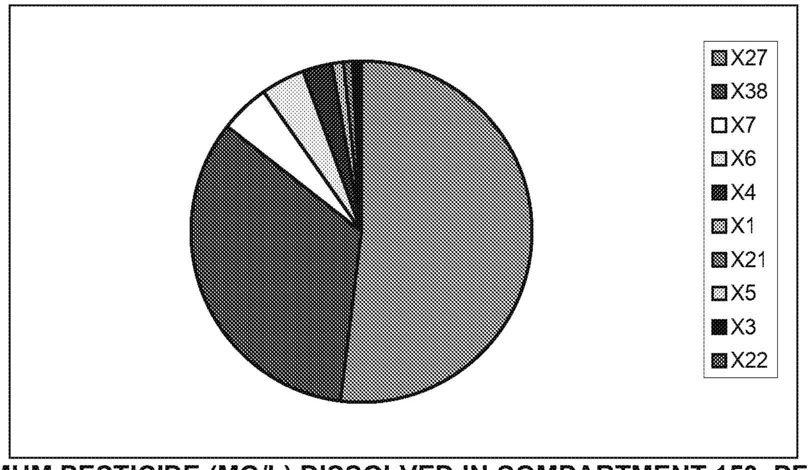
Quasi-global analysis

E/E_{max} for MAXIMUM TOTAL PESTICIDE (MG/KG) IN COMPARTMENT 150, PF =10%

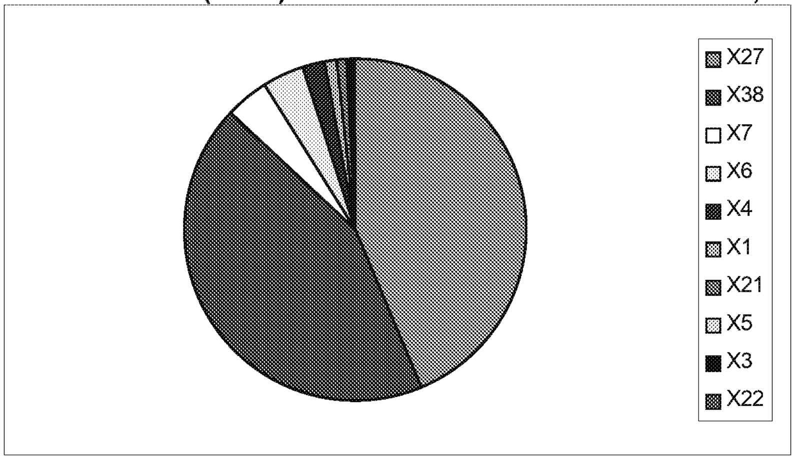


Example of data summarization of constrained analysis.

$|E/E_{max}|$ for MAXIMUM TOTAL PESTICIDE (MG/KG) IN COMPARTMENT 150, PF =1%



$|E/E_{max}|$ for MAXIMUM PESTICIDE (MG/L) DISSOLVED IN COMPARTMENT 150, PF=1%



$|E/E_{max}|$ for TOTAL DISP. FLUX (MG/HA/YEAR) AT SOIL CORE DEPTH, PF=1%